

Exact Ground State of Strongly Correlated Electron Systems from Symmetry-Entangled Wave-Functions

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The four-site Hubbard model is considered from the exact diagonalisation and variational method points of view. It is shown that the exact ground-state can be recovered by a symmetry projected Slater determinant, irrespective of the interaction strength. This is in contrast to the Gutzwiller wave-function, which is calculated as well.

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1 Introduction

The intriguing properties of transition metal oxides have a long history, perhaps starting with the pioneering work of de Boer and Verwey on systems with partially filled and with completely filled 3d-bands [1]. Since then, tremendous efforts have been devoted to the study of transition metal oxides, especially in the form of perovskites ABO_3 , with A being, e. g., La, Sr or a mixture of both of them, and B any transition metal. As reviewed by Imada *et. al.* [2], numerous phase transitions have been discovered, especially towards magnetic and superconducting states [3], as well as the Mott metal-to-insulator transition. Arising in systems with partially filled bands, it points towards the relevance of electronic correlations. Examples are provided by RTiO_3 (see, e.g., [4]) and RNiO_3 (see, e.g., [5] for a review), with R being a rare earth. Furthermore, the colossal magnetoresistance (see, e.g., [6]) and large thermopower (see, e.g., [7]) have attracted considerable interest, too.

The transition metal oxides family is richer, and interest in systems exhibiting application-oriented properties immensely grew in recent years. This is especially true for high- T_c superconductors (see, e.g., [8,9]), transparent conducting oxides (see, e.g., [10]), quantum criticality (see, e.g., [11]), and high capacitance heterostructures [12], to quote a few. In addition, they also entail fascinating phenomena such as superconductivity at the interface of two insulators [13], peculiar magnetism in low dimensional systems [14], high temperature ferromagnetism in vanadate superlattices [15], all of them providing a strong challenge to investigate these systems from the theory side. Yet, one may fairly say that current theoretical approaches meet with severe difficulties when studying the models which describe these systems. Indeed, the tool which is best mastered (perturbation theory), badly fails when the Coulomb interaction is sufficiently strong, thereby calling for alternative approaches.

The microscopic model for interaction driven properties which has received the largest amount of attention is certainly the Hubbard model [16–18], especially after Anderson’s proposal that the key properties of high- T_c superconductors are embodied in it or in the t-J model [19]. The Hubbard model describes an interacting many-body system which cannot be solved analytically, except for dimension $d = 1$ [20], or in the limit of large spacial dimensions [21–23].

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In two dimensions, consensus has been reached at half-filling only: the interaction strength drives a Mott transition [24] to an insulator with long-ranged antiferromagnetic (AF) order [25]. The consequences of (hole) doping remain controversial: The debate focuses on whether the ground-state supports charge inhomogeneities or unconventional fermion-pair condensates and, if so, how their order parameters are intertwined with magnetic properties. Even though numerous many-body techniques have been applied, only a partial answer could be obtained. As reviewed in [26], they are, e. g., cluster extensions [27] of the dynamical mean-field theory [23], the two-particle self-consistent approximation [28], Gutzwiller variational schemes [29], or slave-boson approaches [30, 31]. Standard quantum Monte Carlo simulations (QMC) are also restricted [32] owing to the notorious sign problem that is particularly severe for doped Hubbard models.

An alternative approach with unrestricted symmetry projected wave-functions has been recently introduced. This symmetry-entangled mean-field (SEMF) theory is variational [33], and has been shown to be exact for a two-site cluster, sharing this property with the Gutzwiller wave-function (GWF). In addition, excellent agreement with exact diagonalisation data on 4×4 clusters has been obtained [34]. This then raises the question of whether the SEMF could be exact for clusters made of more than two sites, which provides the purpose of this paper. It is organised as follows: We first summarise in Section 2 the exact diagonalisation procedure to the calculation of the ground-state of the Hubbard model on a 2×2 cluster which we determine. We then present the principles of the SEMF in Section 3 and work out the wave-function obtained after restoration of the spin rotational invariance. For comparison, we also determine the Gutzwiller wave-function as well as the Hartree-Fock wave-function. Finally, in Section 4 we calculate the SEMF wave-function obtained after spin and total momentum projection, and we show that the exact ground-state energy is recovered for arbitrary interaction strength. Our work is summarised in Section 5.

2 Exact diagonalisation for the ground-state

In this work we consider the Hubbard Model on four sites $i \in \{a, b, c, d\}$ as depicted in Fig. 1. We write the Hamiltonian in the form

$$\mathcal{H} = -\frac{t}{2} \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \quad (1)$$

Note that the unusual factor $\frac{1}{2}$ for the hopping amplitude is simply introduced to avoid double counting following from the periodic boundary conditions (PBC) we use. This Hamiltonian is invariant under both continuous and discrete symmetry operations. They involve the $SU(2)$ spin rotational symmetry, as well as translational symmetry and C_{4v} lattice transformations. In addition, at half-filling, the Hamiltonian Eq. (1) possesses $SU(2)$ charge rotational symmetry. As it turns out that this symmetry is not needed to obtain the exact ground-state in the SEMF approach, it will be discarded.

According to previous studies [35, 36] the ground-state is characterised by zero total spin, zero total momentum and d-wave symmetry. A convenient basis to the calculation of the ground-state may be found starting from a state with two doubly occupied sites that is symmetrised according to the above quantum numbers. The other basis states are obtained by repeatedly applying the hopping operator. Thus, we end with a three-dimensional subspace spanned by the following vectors:

$$\begin{aligned} |1\rangle &= \frac{1}{2} \left(\Delta_a^\dagger - \Delta_d^\dagger \right) \left(\Delta_b^\dagger - \Delta_c^\dagger \right) |0\rangle \\ |2\rangle &= \frac{1}{4} \left[\left(\Delta_a^\dagger + \Delta_b^\dagger \right) \left(c_{c\uparrow}^\dagger c_{d\downarrow}^\dagger - c_{c\downarrow}^\dagger c_{d\uparrow}^\dagger \right) - \left(\Delta_a^\dagger + \Delta_c^\dagger \right) \left(c_{b\uparrow}^\dagger c_{d\downarrow}^\dagger - c_{b\downarrow}^\dagger c_{d\uparrow}^\dagger \right) \right. \\ &\quad \left. - \left(\Delta_b^\dagger + \Delta_d^\dagger \right) \left(c_{a\uparrow}^\dagger c_{c\downarrow}^\dagger - c_{a\downarrow}^\dagger c_{c\uparrow}^\dagger \right) + \left(\Delta_c^\dagger + \Delta_d^\dagger \right) \left(c_{a\uparrow}^\dagger c_{b\downarrow}^\dagger - c_{a\downarrow}^\dagger c_{b\uparrow}^\dagger \right) \right] |0\rangle \\ |3\rangle &= \frac{1}{2\sqrt{3}} \left[c_{a\uparrow}^\dagger c_{b\uparrow}^\dagger c_{c\downarrow}^\dagger c_{d\downarrow}^\dagger + c_{a\downarrow}^\dagger c_{b\uparrow}^\dagger c_{c\downarrow}^\dagger c_{d\uparrow}^\dagger + c_{a\downarrow}^\dagger c_{b\downarrow}^\dagger c_{c\uparrow}^\dagger c_{d\uparrow}^\dagger + c_{a\uparrow}^\dagger c_{b\downarrow}^\dagger c_{c\uparrow}^\dagger c_{d\downarrow}^\dagger \right. \\ &\quad \left. - 2 \left(c_{a\uparrow}^\dagger c_{b\downarrow}^\dagger c_{c\downarrow}^\dagger c_{d\uparrow}^\dagger + c_{a\downarrow}^\dagger c_{b\uparrow}^\dagger c_{c\uparrow}^\dagger c_{d\downarrow}^\dagger \right) \right] |0\rangle \end{aligned} \quad (2)$$

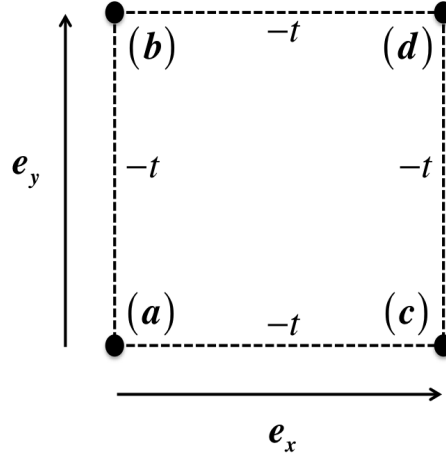


Fig. 1 Labelling of the sites for the Hubbard model on the 2×2 cluster.

where we introduced the short-hand notation $\Delta_i^\dagger \equiv c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$. In this basis the Hamiltonian matrix reads:

$$H = \begin{pmatrix} 2U & 2t & 0 \\ 2t & U & -2\sqrt{3}t \\ 0 & -2\sqrt{3}t & 0 \end{pmatrix} \quad (3)$$

In order to determine the eigenvalues E_k it is convenient to write:

$$E \equiv U - 4t\zeta. \quad (4)$$

ζ then satisfies to a cubic equation in depressed form:

$$16t^3\zeta^3 - \zeta(16t^2 + U^2)t - 2t^2U = 0. \quad (5)$$

Eq. (5) may be solved using Cardano's formula, and the eigenvalues of the Hamiltonian matrix Eq. (3) finally read:

$$E_k = U - 2\sqrt{\frac{16t^2 + U^2}{3}} \cos\left(\frac{\beta - 2k\pi}{3}\right) \quad (6)$$

with $k = 0, 1, 2$, and

$$\cos\beta = 4t^2U \left(\frac{3}{16t^2 + U^2}\right)^{\frac{3}{2}}. \quad (7)$$

The ground-state corresponds to $k = 0$.

The Hamiltonian Eq. (1) also corresponds to the Hubbard Model on a four-site chain with PBC. Note that the d-wave character of the ground-state on the 2×2 cluster maps onto a total momentum $K = \pi$ for the chain. Then, the solution Eqs. (6-7) reproduces the results obtained in the 1D case [37, 38].

3 Principles of the SEMF approach for the 2×2 cluster

Symmetry breaking wave-functions with assumed magnetic, charge or superconducting orders are usually considered in variational treatments of the Hubbard model [39]. However, on finite-size clusters, Hamiltonian symmetries must be restored by quantum fluctuations and substantial energy improvements can be

obtained by quantum number projection on top of these states. An illustration with the Gutzwiller wavefunction can be found in [40]. Indeed, symmetry restoration leads to coherent superpositions of symmetry related states that induce correlations. The SEMF approach follows such a strategy to approximate low-lying eigenstates of the Hubbard model. Up to now, the method works at the Hartree-Fock level and gives the optimal Slater determinant minimising the energy *after* symmetry projection. First attempts for the spectroscopy of Hubbard chains [41] and square clusters up to 36 sites have been performed with reliable results [42]. By reformulating the stationarity of the projected energy as a mean-field like equation, SEMF simulations on larger cells and with all symmetries of the Hubbard model have revealed an intriguing interplay of spin, charge and pairing correlations in the hole doped region [33].

3.1 Restoration of spin-rotational invariance

One of the most attractive features of the SEMF approximation relies on the ability to perform an unbiased energy minimisation, *i.e.* to consider totally unrestricted Slater determinants. However, we here focus on analytical SEMF solutions and thus follow conventional calculations with projected wave-functions by constraining the variational subspace to exhibit a relevant order. At half-filling, an antiferromagnetic Slater determinant $|\Phi_{\text{ref}}\rangle$ is considered. For the 2×2 cluster, we assume a positive magnetisation m on sites a and d, and the opposite magnetisation on sites b and c. In each spin sector σ , the two occupied orbitals are simply obtained as the lowest energy eigenstates of the effective one-body Hamiltonian

$$h_{\sigma}^{\text{ref}}[m] = \begin{pmatrix} \frac{U}{2}(1 - \sigma m) & -t & -t & 0 \\ -t & \frac{U}{2}(1 + \sigma m) & 0 & -t \\ -t & 0 & \frac{U}{2}(1 + \sigma m) & -t \\ 0 & -t & -t & \frac{U}{2}(1 - \sigma m) \end{pmatrix}. \quad (8)$$

For our purpose, it is convenient to introduce

$$\begin{aligned} \tilde{m} &= \frac{Um}{2t} \\ \cos(2\varphi) &= \frac{\tilde{m}}{\sqrt{4 + \tilde{m}^2}} \\ \sin(2\varphi) &= \frac{2}{\sqrt{4 + \tilde{m}^2}} \end{aligned} \quad (9)$$

in terms of which the four-electron state $|\Phi_{\text{ref}}\rangle$ reads:

$$|\Phi_{\text{ref}}\rangle = c_{\phi_1\uparrow}^{\dagger} c_{\phi_2\uparrow}^{\dagger} c_{\phi_3\downarrow}^{\dagger} c_{\phi_4\downarrow}^{\dagger} |0\rangle \quad (10)$$

with

$$\begin{aligned} |\phi_1\rangle &= \frac{1}{\sqrt{2}} (|a\rangle - |d\rangle) \\ |\phi_2\rangle &= \frac{1}{\sqrt{2}} (\cos(\varphi)|a\rangle + \sin(\varphi)|b\rangle + \sin(\varphi)|c\rangle + \cos(\varphi)|d\rangle) \\ |\phi_3\rangle &= \frac{1}{\sqrt{2}} (|b\rangle - |c\rangle) \\ |\phi_4\rangle &= \frac{1}{\sqrt{2}} (\sin(\varphi)|a\rangle + \cos(\varphi)|b\rangle + \cos(\varphi)|c\rangle + \sin(\varphi)|d\rangle) \end{aligned} \quad (11)$$

In SEMF, one introduces a symmetry adapted mean-field state $|\Psi\rangle = \mathcal{P}^{(\Gamma)} |\Phi_{\text{ref}}\rangle$ where $\mathcal{P}^{(\Gamma)}$ is a projector on the subspace with quantum numbers Γ . We first limit ourselves to the restoration of spin rotational invariance for which the singlet projection can be achieved by [43]

$$\mathcal{P}^{(S=0)} = \frac{1}{8\pi^2} \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin \beta \int_0^{2\pi} d\gamma R(\alpha, \beta, \gamma) \quad (12)$$

where $R(\alpha, \beta, \gamma) = e^{i\alpha S_z} e^{i\beta S_y} e^{i\gamma S_z}$ is the Euler angles (α, β, γ) parameterisation of rotations (with S the total spin observable). The unnormalised $S = 0$ component of the AF state is then easily obtained and may be written as a linear combination of the basis vectors $|1\rangle, |2\rangle, |3\rangle$ Eq. (2) spanning the subspace of the exact ground-state :

$$|\Psi\rangle = \sin^2(\varphi)|1\rangle - \sin(2\varphi)|2\rangle - \frac{1 + \cos^2(\varphi)}{\sqrt{3}}|3\rangle \quad (13)$$

Indeed, this result reflects unbroken symmetries of the AF reference state. For instance, one can immediately check that $|\Phi_{\text{ref}}\rangle$ is invariant under a spin-rotation around the y-axis by an angle π combined with a translation T_y by one lattice spacing along the y-direction. Therefore, after performing all spin rotations and integrating over the Euler angles, the resulting $S = 0$ vector is simultaneously translational invariant:

$$\begin{aligned} T_y |\Psi\rangle &= \frac{1}{4\pi} \int_0^{2\pi} d\alpha e^{i\alpha S_z} \int_0^\pi d\beta \sin \beta e^{i\beta S_y} T_y |\Phi_{\text{ref}}\rangle \\ &= \frac{1}{4\pi} \int_0^{2\pi} d\alpha' e^{-i(\alpha' - 2\pi) S_z} \int_0^\pi d\beta' \sin(\pi - \beta') e^{-i\beta' S_y} e^{i\pi S_y} T_y |\Phi_{\text{ref}}\rangle \\ &= e^{2i\pi S_z} \mathcal{P}^{(S=0)} |\Phi_{\text{ref}}\rangle = |\Psi\rangle \end{aligned} \quad (14)$$

where we used the hermiticity of the projector Eq. (12). With the help of the Hamiltonian matrix Eq. (3) in the subspace $|1\rangle, |2\rangle$, and $|3\rangle$, one is left with the following average energy $E^{(S=0)}$ in the SEMF state $|\Psi\rangle$:

$$\langle \mathcal{H} \rangle_{\mathcal{P}^{(S=0)} \Phi_{\text{ref}}} = \frac{\frac{3}{8}U (5 - 4 \cos(2\varphi) - \cos(4\varphi)) - 12t \sin(2\varphi)}{2 + \sin^2(2\varphi)} \quad (15)$$

Its minimisation with respect to φ yields a cubic equation for the dimensionless staggered magnetisation \tilde{m} :

$$2\tilde{m}t(2 + \tilde{m}^2) - U(3 + \tilde{m}^2) = 0 \quad (16)$$

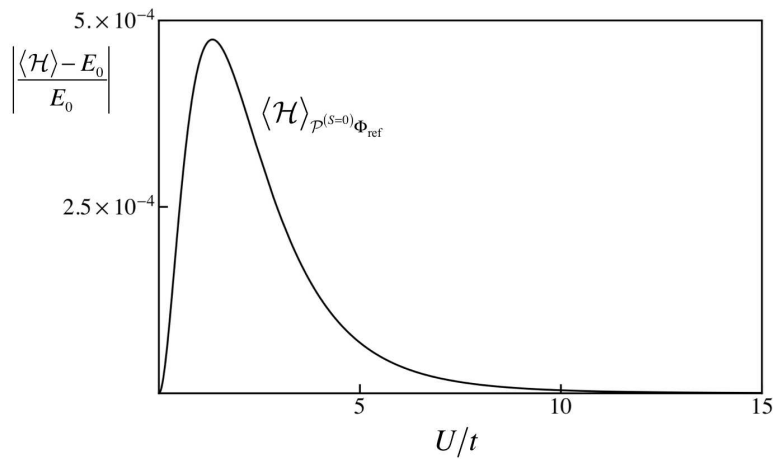


Fig. 2 Ground-state energy from spin singlet projected SEMF.

Comparison of the resulting energy to the exact solution is performed in Fig. 2. The agreement is obviously excellent for any on-site interaction, but the SEMF approach limited to the spin singlet projection is not exact.

3.2 Comparison with the conventional Gutzwiller wave-function

Let us now proceed to the usual variational calculation with the Gutzwiller projector

$$\mathcal{P}_G = \Pi_i \left(1 + (g - 1)n_{i,\uparrow}n_{i,\downarrow} \right) \quad (17)$$

to reduce the weights of configurations with double occupancy in the AF reference state. Thus, one aims at minimising :

$$\langle \mathcal{H} \rangle(\varphi, g) \equiv \frac{\langle \Phi_{\text{ref}} | \mathcal{P}_G \mathcal{H} \mathcal{P}_G | \Phi_{\text{ref}} \rangle}{\langle \Phi_{\text{ref}} | \mathcal{P}_G \mathcal{P}_G | \Phi_{\text{ref}} \rangle} \quad (18)$$

with respect to φ and g . While the evaluation of the norm of the projected wave-function and the expectation value of the interaction energy is straightforward, the one of the kinetic energy is more tedious. Yet, symmetries of the AF background greatly simplify the calculation since all hopping contributions are equal. For instance, from the invariance of $|\Phi_{\text{ref}}\rangle$ under the product $U_y = T_y R(0, \pi, 0)$, one has:

$$\begin{aligned} \langle \Phi_{\text{ref}} | \mathcal{P}_G c_{a\uparrow}^\dagger c_{c\uparrow} \mathcal{P}_G | \Phi_{\text{ref}} \rangle &= \langle \Phi_{\text{ref}} | \mathcal{P}_G U_y^\dagger c_{a\uparrow}^\dagger c_{c\uparrow} U_y \mathcal{P}_G | \Phi_{\text{ref}} \rangle \\ &= \langle \Phi_{\text{ref}} | \mathcal{P}_G c_{b\downarrow}^\dagger c_{d\downarrow} \mathcal{P}_G | \Phi_{\text{ref}} \rangle \end{aligned} \quad (19)$$

where we have used the invariance of the Gutzwiller operator under symmetry transformations of the Hamiltonian. The average energy (12) is finally obtained as:

$$\langle \mathcal{H} \rangle_{\mathcal{P}_G \Phi_{\text{ref}}} = \frac{[-8tg \sin(\varphi) \cos(\varphi) + 2Ug^2 \sin^2(\varphi)] [(1+g)^2 \sin^2(\varphi) + 4 \cos^2(\varphi)]}{4 \cos^4(\varphi) + 8g^2 \cos^2(\varphi) \sin^2(\varphi) + (1+g^2)^2 \sin^4(\varphi)} \quad (20)$$

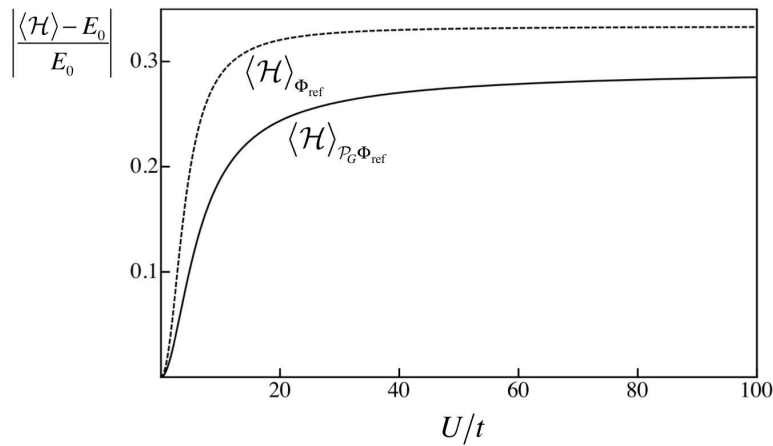


Fig. 3 Ground-state energy from antiferromagnetic Gutzwiller wave-function (full line) and in mean-field theory (dashed line), relative to the exact one.

Minimising Eq. (20) with respect to g and φ reveals that the relative energy difference with the exact solution increases with U and saturates to 28% for $U \rightarrow \infty$ as shown in Fig. 3. Nevertheless, the Gutzwiller projection improves the simple Hartree-Fock approximation which is recovered by imposing the staggered magnetisation m to solve the self-consistency condition $m = \langle n_{a\uparrow} - n_{a\downarrow} \rangle_{\Phi_{\text{ref}}}$. This relation is equivalent to require a zero derivative of $\langle \mathcal{H} \rangle_{\Phi_{\text{ref}}}$ with respect to m . The energy obtained with such a mean-field solution is also displayed in Fig. 3 and gives a relative error of 33% in the strong coupling limit of the Hubbard model.

4 The exact ground-state as a symmetry projected wave-function

In the spirit of the SEMF methodology, breaking symmetries in the underlying reference state followed by their restoration is a way to recover the small part of the correlation energy that cannot be reached by the only projection onto the spin-singlet subspace. We consider here a scheme obtained by adding a bond-spin contribution to an antiferromagnetic order, as depicted in Fig. 4. As a result, the Slater determinant $|\Phi_{\text{ref}}\rangle$ is built from the lowest energy eigenstates of the mean-field like Hamiltonian:

$$h_{\sigma}^{\text{ref}}[m, s] = \begin{pmatrix} \frac{U}{2}(1 - \sigma m) & -t(1 + \sigma s) & -t(1 + \sigma s) & 0 \\ -t(1 + \sigma s) & \frac{U}{2}(1 + \sigma m) & 0 & -t(1 - \sigma s) \\ -t(1 + \sigma s) & 0 & \frac{U}{2}(1 + \sigma m) & -t(1 - \sigma s) \\ 0 & -t(1 - \sigma s) & -t(1 - \sigma s) & \frac{U}{2}(1 - \sigma m) \end{pmatrix}. \quad (21)$$

The SEMF variational ansatz then results from the projection on zero-spin and total momentum $\mathbf{K} = (0, 0)$:

$$|\Psi\rangle = \mathcal{P}^{(\mathbf{K}=0)} \mathcal{P}^{(S=0)} |\Phi_{\text{ref}}\rangle \quad (22)$$

where $P^{(\mathbf{K}=0)} = \frac{1}{4}(\mathbf{I} + T_x + T_y + T_{x+y})$ ensures the invariance under translations T_x, T_y, T_{x+y} by one lattice spacing along the directions $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_x + \mathbf{e}_y$ [43]. Through similar steps as for spin projection, the SEMF energy is given by

$$E^{(S=0, \mathbf{K}=0)} = \frac{3(1 + s^2)}{2} \times \frac{-8t(\tilde{m}s^2 + (2 + s^2)A) + U(1 + s^2)(6 + \tilde{m}^2 + 2s^2 - \tilde{m}A)}{\tilde{m}s^2A + 2(1 + s^2)(6 + 6s^2 + s^4) + \tilde{m}^2(2 + 3s^2 + 2s^4)} \quad (23)$$

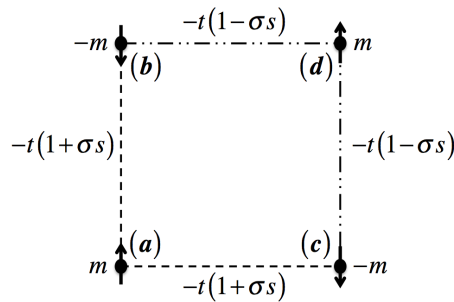


Fig. 4 Mean-field like scheme defining the reference Slater determinant for the SEMF approach with spin and total momentum projection.

with $A \equiv \sqrt{4(1+s^2) + \tilde{m}^2}$. In order to solve analytically the minimum equations it is convenient to introduce new variables, ξ and η . They are defined as:

$$\begin{aligned}\xi &\equiv \frac{2(2+s^2) + \tilde{m} \left(\tilde{m} + \sqrt{4(1+s^2) + \tilde{m}^2} \right)}{2 \left(\tilde{m} + \sqrt{4(1+s^2) + \tilde{m}^2} \right)} \\ \eta &\equiv \frac{2}{\sqrt{4(1+s^2) + \tilde{m}^2} - \tilde{m}},\end{aligned}\quad (24)$$

and allow to cast the energy (23) in the form

$$E^{(S=0, \mathbf{K}=0)} = \frac{3}{2} \frac{-16\xi\eta^2 t + U(1+2\eta^2)}{4\xi^2\eta^2 + 3\eta^2 - 2\xi\eta + 1}. \quad (25)$$

Minimisation with respect to ξ and η yields:

$$\begin{aligned}\xi^2 4\eta(4\eta t - U) - \xi((2\eta^2 - 1)U + 16\eta) &= U\eta \\ \xi^2 32\eta^3 t - 4\xi U\eta(2\eta^2 + 1) &= 8\eta t(3\eta^2 + 1) - U(2\eta^2 + 1).\end{aligned}\quad (26)$$

Eq. (26) may be viewed as a linear system of equations in ξ and ξ^2 that is easily solved to express these variables in terms of η , *i.e.* $\xi = f(\eta)$, $\xi^2 = g(\eta)$. Therefore, the relation $g(\eta) - f(\eta)^2 = 0$ has to be satisfied, which can be factorised into

$$\begin{aligned}&[8\eta^3 t^2 - 6\eta^2 tU + \eta(U^2 - 8t^2) + tU] \times \\ &[4\eta^4(48t^2 + U^2) - 16\eta^3 tU + 4\eta^2(16t^2 + U^2) - 8\eta tU + U^2] = 0\end{aligned}\quad (27)$$

The quartic factor $Q(\eta)$ as a function of $\eta > 0$ is strictly positive for any interaction strength. Indeed, $Q(0) = U^2$ and Q goes to infinity with η which proves the result in the case of a monotonic evolution. Otherwise, the value $Q(\eta_0)$ at an extremum point η_0 can be obtained from the remainder of the Euclidean division of the polynomial Q by its derivative :

$$Q(\eta_0) = \frac{2\eta_0^2(768t^4 + 58t^2U^2 + U^4) - 4\eta_0 tU(64t^2 + U^2) + U^2(46t^2 + U^2)}{48t^2 + U^2} \quad (28)$$

Since the discriminant of the quadratic numerator is strictly negative, $Q(\eta_0) > 0$ and so $Q(\eta) > 0$ even for non-monotonic behaviour. Finally, the SEMF energy for $S = 0$ and $\mathbf{K} = (0, 0)$ is minimised if and only if η is a root of the cubic factor in Eq. (27). In this case, the difference $\eta - \xi = \eta - f(\eta)$ simplifies to the interaction, up to a constant:

$$\eta - \xi = \frac{U}{4t} \quad (29)$$

Thus, the cubic equation for η turns into a similar equation in terms of ξ :

$$16t^2\xi^3 - \xi(16t^2 + U^2) - 2tU = 0 \quad (30)$$

This relation must be satisfied for the projected energy Eq. (25) to reach its minimum, given by

$$E_{\min}^{(s=0, \mathbf{K}=0)} = U - 4\xi t \quad (31)$$

We recover exactly Eq. (4) and Eq. (5) obtained in Section 2 after direct diagonalisation of the Hamiltonian matrix. Note that the result is valid for arbitrary interaction strength. This SEMF derivation provides an alternative view of the exact ground-state in terms of a one-parameter symmetry restored Slater determinant.

5 Conclusion

In this work we showed analytically that conventional Hartree-Fock approximations can be greatly improved to account for strong electronic correlations as long as the variational ansatz is enhanced by symmetry projections. For the 2×2 cluster, we demonstrated that restoring the spin-rotational invariance leads to an almost exact description. Furthermore, we established that the more symmetry breakings in the underlying Slater determinant followed by their restoration, the better the SEMF approach will be. Specifically, spin-singlet and total momentum are sufficient to recover the exact ground-state for any interaction strength. Combined with previous numerical results on larger cells [33], the present work highlights the SEMF method as a reliable starting point to elucidate correlations that spontaneously emerge from the Hubbard model at low energy.

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